

# Shadow bands, gap and pseudogaps in high- $T_c$ superconductors.

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Within the framework of the Charge Density Wave Quantum Critical Point (*CDW-QCP*) scenario for high- $T_c$  superconductors (HTCS), we introduce a model for tight-binding electrons coupled to quasi-critical fluctuations. In the normal state our model reproduces features of the Fermi Surface (FS) observed in *ARPES* measurements on optimally doped Bi2212, such as the anisotropic suppression of spectral weight around the  $M$  points of the Brillouin zone. The spectral density is characterized by a transfer of spectral weight from the main quasi-particle peak to dispersing shadow peaks which originate branches of a shadow FS. In the superconducting state our model reproduces the  $d$ -wave symmetry of the gap parameter, which results from a balance between small- $q$  attraction and large- $q$  repulsion. The gap parameter is enhanced due to cooperative effects of charge and spin fluctuations.

Recently it has been proposed that the anomalous normal-state and the superconducting properties of HTSC are the natural consequence of the existence of a *CDW-QCP* near optimal doping [1-4] which gives rise to large charge fluctuations in the electronic system. The dynamical charge segregation in hole-poor and hole-rich regions induces antiferromagnetic spin fluctuations even at optimal doping. When the electrons are coupled to quasi-critical charge and spin fluctuations a strongly momentum and frequency dependent electron-electron interaction appears.

We consider a model of tight binding electrons coupled with charge and spin fluctuations

$$H = \sum_{k,\sigma} \xi_k c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_{j=0}^4 g_j \sum_{k,q,\sigma,\sigma'} c_{k,\sigma}^\dagger c_{k+q,\sigma'} \tau_{\sigma,\sigma'}^j S_{-q}^j$$

where  $\xi_k = -2t(\cos k_x + \cos k_y + \alpha \cos k_x \cos k_y) - \mu$  (commonly used values for Bi2212 being  $t = 0.2eV$ ,  $\alpha = -0.5$  and  $\mu = -0.18eV$  to fix the hole doping  $\delta = 0.17$ ),  $j = 0$  for charge and  $j = 1, 2, 3$  for spin.

The fluctuating modes are characterized by effective susceptibilities

$$\chi_{ij}(q, \omega) = \delta_{ij} \frac{A_j}{\Omega_j(q) - i\omega}$$

where  $\Omega_j(q) = t_j^* + \bar{\omega}_j [2 - \cos(q - Q_j)_x - \cos(q - Q_j)_y]$ ,  $t_j^*$  is a mass term depending on the distance from the *QCP*,  $\bar{\omega}_j$  is a characteristic energy scale associated with the damping of the fluctuations, and the critical wavevector for spin fluctuations is  $Q_s \simeq (\pi; \pi)$  while for charge fluctuations we take  $Q_c = (0.4\pi; -0.4\pi)$  as suggested by

recent experimental results [5]. The above expression for the effective spin susceptibility was suggested to fit NMR results in the region of overdamped spin waves [6]. The form of the charge susceptibility results from a slave-boson calculation within the Hubbard-Holstein model with long-range Coulombic interaction, close to the CDW instability [1].

We calculate first order selfenergy corrections to the quasiparticle spectra. The imaginary part of the self-energy is characterized by peaks corresponding to the energies  $\epsilon \simeq \xi_{k-Q_j}$ ; as  $\xi_{k-Q_j} \rightarrow 0$  the peaks are suppressed while the usual low-energy Fermi-liquid behavior is turned into an anomalous square-root behavior. The peaks in the imaginary part of the selfenergy are responsible for the appearance of shadow peaks in the spectral density

$$A(k, \omega) = \frac{1}{\pi} \frac{|Im\Sigma(k, \omega)|}{[\omega - \xi_k - Re\Sigma(k, \omega)]^2 + [Im\Sigma(k, \omega)]^2}$$

To compare with the *ARPES* experiments in [5] we describe the FS associating to each  $k$ -point the spectral weight  $p_k$  of occupied states within an energy window  $[-W, W]$  (a typical experimental value is  $2W = 50meV$ ), i.e.

$$p_k = \int_{-W}^W d\omega A(k, \omega) f(\omega).$$

Spin fluctuations by themselves would preserve the full symmetry of the FS due to the peculiar commensurability of the critical wavevector  $Q_s = (\pi; \pi)$ . The main effects of the coupling to spin fluctuations is a symmetric suppression of spectral weight around the  $M$  points of the Brillouin zone, and the appearance of weak "hole pockets" around the points  $(\pm\pi/2; \pm\pi/2)$  due to a transfer of spectral weight to lower energies at the shadow FS. Along the  $\Gamma M$  direction the main quasiparticle peak is suppressed and a broader shadow peak appears at the  $M$  point below the Fermi energy.

In Bi2212 the experimentally observed FS [2] indicates that the mirror symmetry with respect the  $\Gamma X(Y)$  axes is preserved, whereas the symmetry with respect to the  $\Gamma M(M_1)$  axes is broken, suggesting a  $Q_c$  directed along the  $\Gamma X(Y)$  directions. A charge-fluctuation mode with a diagonal  $Q_c$  may reproduce these features, the main effect of charge fluctuations being, indeed, an asymmetric modulation of spectral weight around the  $M(M_1)$  points. When both modes are taken into account, the suppression of spectral weight around the  $M$  points due to spin fluctuations is modulated by charge fluctuations leading

to an asymmetric distribution as experimentally observed (Fig. 1). Moreover the broad structure at the  $M$  point below the Fermi energy, due to spin fluctuations, persists.

We then consider the static effective interaction in the Cooper channel  $\Gamma_{eff}(q) = g_s^2 \chi_s(q, \omega = 0) - g_c^2 \chi_c(q, \omega = 0)$ , and we solve the  $BCS$  equation

$$\Delta(k) = -\frac{1}{N} \sum_p \Gamma_{eff}(k-p) \frac{\tanh \frac{\varepsilon_p}{2T}}{2\varepsilon_p} \Delta(p)$$

where  $\varepsilon_p^2 = \xi_p^2 + \Delta(p)^2$  and  $\Delta(k)$  is the gap parameter. The cooperative charge and spin fluctuations enhance the  $d_{x^2-y^2}$ -wave gap parameter leading to larger values with respect to the charge or spin fluctuations when considered separately. The  $k$  dependence of the gap is due to an interplay between the band structure and the effective interaction. The modulus of the gap tends to follow the local density of states for small  $q$  attraction. For singular quasiparticle interactions the gap has local maxima at the points where  $\xi_k = \xi_{k-Q_j} = 0$  (hot spots). We obtain two different behaviors for  $\Delta(k)$  in the  $d_{x^2-y^2}$  channel according to vertical or diagonal  $Q_c$  directions (Fig. 2).

In the underdoped region, the charge fluctuation become critical near the  $T_{CDW}$  line, where  $CDW$  transition would occur in the absence of pairing and the attractive fluctuations lead to local pairs with pseudogap opening. The stabilizing effect of local superconducting order, with respect to the  $CDW$  instability, is introduced via the local gap. In this situation we reproduce the general trend of the temperature dependence of the pseudogap.

In **conclusion**, within the framework of the  $CDW$ - $QCP$  scenario for HTSC, we have investigated the properties of a model for electrons coupled with both charge and spin quasi-critical fluctuations.

In the normal state we reproduce features of the FS as observed in recent *ARPES* measurements [5,7]. In particular we recover an anisotropic suppression of spectral weight around the  $M$  points of the Brillouin zone and shadow features associated to charge and spin fluctuations.

In the superconducting state we obtain a  $d$ -wave superconducting gap as a result of the balance between repulsion (spin fluctuations) and attraction (charge fluctuations) between quasiparticles. We find that the gap parameter and the critical temperature are enhanced due to the cooperative effects of charge and spin fluctuations.

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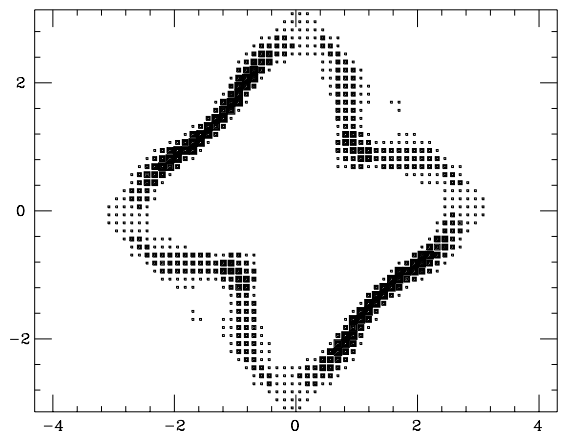


FIG. 1. Fermi surface in presence of charge and spin fluctuations with  $Q_c = (0.4\pi; -0.4\pi)$  and  $Q_s = (\pi; \pi)$ .

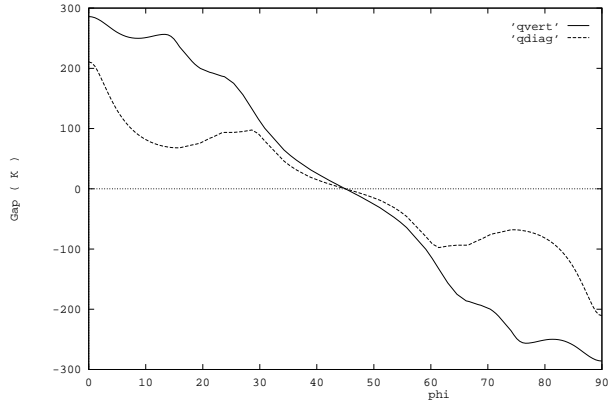


FIG. 2. Gap parameter in presence of charge and spin fluctuations with  $Q_c = (0.4\pi; 0)$  (solid line) or  $Q_c = (0.4\pi; -0.4\pi)$  (dashed line) and  $Q_s = (\pi, \pi)$ .